NM_EXEC_3

1) Determinant of matrix factorizations

a) LU factorization

So for a lower triangular matrix:

$$L = \begin{pmatrix} 1 & 0 & \dots & 0 \\ l_{21} & 1 & \dots & 0 \\ \vdots & \dots & 1 & 0 \\ l_{n,1} & \dots & \dots & 1 \end{pmatrix}$$

Therefore $\det L = \prod_{i=1}^{n} l_{ii}$

And for an upper triangle matrix:

$$U = \begin{pmatrix} 1 & u_{12} & \dots & u_{1n} \\ 0 & 1 & \dots & u_{2n} \\ \vdots & \dots & \ddots & u_{kn} \\ 0 & \dots & \dots & 1 \end{pmatrix}$$

Also here $\det U = \prod_{i=1}^{n} u_{ii}$

So in total $\det A = \det L \cdot \det U = \prod_{i=1}^{n} U_{ii}$

b) LU factorization with partial pivoting

$$\begin{aligned} PA &= LU \\ \det(PA) &= \det(LU) \\ \overbrace{\det P}^{\begin{cases} 1 & \text{if even swaps} \\ -1 & \text{if odd swaps} \end{cases}} \cdot \det A &= \overbrace{\det L}^{1} \cdot \det U \\ \det A &= \frac{\det U}{\det P} = \begin{cases} 1 \cdot \det U & \text{if even swaps} \\ -1 \cdot \det U & \text{if odd swaps} \end{cases} \end{aligned}$$

And since U is an upper triangle matrix the determinant is given by its diagonal entries.

c)

Since the matrix needs to be SPD (Self-adjoint positive definite)

$$\begin{aligned} A &= R^* R \\ \det A &= \det(R^* R) \\ &= \det R^* \det R \\ &= (\det R)^* \det R \\ &= |\det R|^2 \end{aligned}$$

d)

$$\begin{aligned}
\det A &= \det Q \cdot \det R \\
&= \det Q \cdot \prod_{i=1}^{n} R_{ii} \\
&= |\det Q| \cdot \prod_{i=1}^{n} R_{ii} \\
&= \begin{cases} 1 \cdot \prod_{i=1}^{n} R_{ii} \\ -1 \cdot \prod_{i=1}^{n} R_{ii} \end{cases}
\end{aligned}$$

We definitely know that the magnitude of $\det Q$ is 1.
$\det Q$ can be a complex number with magnitude 1. So we might have a certain phase but the magnitude is definitely 1.

3) Show that complexity of LU factorization of band matrix is linear in n

Operations needed for processing row k

Dividing by the Pivot $a_{k,k}$

Since each row contains a maximum of $2p+1$ non zero Elements, the number of divisions has an upper bound of $2p+1$

$$\text{Number of Divisions in Step } k = 2p+1$$

Eliminate Entries below the diagonal

Again using the maximum number of non zero entries $2p+1$:
Each row contributes a maximum of $2p+1$ subtractions and $2p+1$ multiplications
Because of the band structure we can put a maximum on the number of rows that need to be eliminated. At each step only rows ranging from $k+1$ to $k+p$ are involved. Because in the other rows the entries are already 0. This means that there are at most p rows involved.

$$\text{Number of Steps in Elmination } = p \cdot (4p+2) = 4p^2 + 2p$$

Total Operations in Step k

$$\text{Total Operations in Step } k = 2p + 1 + 4p^2 + 2p = 4p^2 + 4p + 1$$

Total Operations

Since we are processing n rows the total number of flops is bound by:

$$\text{Total Amount of Operations} \leq n \cdot (4p^2 + 4p + 1)$$

Which scales linear with n

Task

4) Cholesky factorization of:

$$A = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix}$$

General Formulas

Given:

$$l_{k,i} = \frac{a_{k,i} - \sum_{j=1}^{i-1} l_{ij} \cdot l_{kj}}{l_{ii}}$$

and

$$l_{kk} = \sqrt{a_{kk} - \sum_{j=1}^{k-1} l_{kj}^2}$$

Step-by-Step Calculation

1. Calculate l_{11}

$$l_{11} = \sqrt{a_{11}} = \sqrt{2}$$

2. Calculate l_{21}

$$l_{21} = \frac{a_{21}}{l_{11}} = \frac{1}{\sqrt{2}}$$

3. Calculate l_{22}

$$l_{22} = \sqrt{a_{22} - l_{21}^2} = \sqrt{2 - \frac{1}{2}} = \sqrt{1.5} = \sqrt{\frac{3}{2}} = \frac{\sqrt{6}}{2}$$

4. Calculate l_{31}

$$l_{31} = \frac{a_{31}}{l_{11}} = 0$$

5. Calculate l_{32}

$$l_{32} = \frac{a_{32} - l_{31} \cdot l_{21}}{l_{22}} = \frac{1 - 0}{\frac{\sqrt{6}}{2}} = \frac{2}{\sqrt{6}} = \frac{\sqrt{6}}{3}$$

6. Calculate l_{33}

$$l_{33} = \sqrt{a_{33} - l_{32}^2} = \sqrt{2 - \left(\frac{\sqrt{6}}{3}\right)^2}$$

$$= \sqrt{2 - \frac{6}{9}} = \sqrt{2 - \frac{2}{3}} = \sqrt{\frac{4}{3}} = \frac{2\sqrt{3}}{3}$$

7. Calculate l_{41}

$$l_{41} = \frac{a_{41}}{l_{11}} = 0$$

8. Calculate l_{42}

$$l_{42} = \frac{a_{42} - l_{41} \cdot l_{21}}{l_{22}} = \frac{0}{\frac{\sqrt{6}}{2}} = 0$$

9. Calculate l_{43}

$$l_{43} = \frac{a_{43} - l_{41} \cdot l_{31} - l_{42} \cdot l_{32}}{l_{33}} = \frac{1 - 0 - 0}{\frac{2\sqrt{3}}{3}} = \frac{3}{2\sqrt{3}} = \frac{\sqrt{3}}{2}$$

10. Calculate l_{44}

$$l_{44} = \sqrt{a_{44} - l_{43}^2} = \sqrt{2 - \left(\frac{\sqrt{3}}{2}\right)^2}$$

$$= \sqrt{2 - \frac{3}{4}} = \sqrt{\frac{5}{4}} = \frac{\sqrt{5}}{2}$$

Final Result for L The Cholesky factor L is:

$$L = \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{\sqrt{6}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{3} & \frac{2\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{\sqrt{5}}{2} \end{pmatrix}$$

5) If $A \in K^{n \times n}$ has a Cholesky factorization then A is SPD

Symmetric/Hermitian

So A has a decomposition like $A = R^* R$

$$A^* = (R^* R)^* = R^* R = A$$

Positive Definiteness

A Matrix is positive definite if, for any non-zero vector $x \in K^n$, we have:

$$\vec{x}^* \vec{A} x > 0$$

$$
\begin{aligned}
\vec{x}^* \vec{A} x &= \vec{x}^*(R^* R)\vec{x} \\
&= (\vec{x}^* R^*)\underbrace{(\vec{R} x)}_{\vec{y}} \\
&= \vec{y}^* \vec{y} = |\vec{y}|^2
\end{aligned}
$$

We know that R is invertible. Therefore $\vec{y} \neq 0$ if $\vec{x} \neq 0$.
And we know for sure that as long as $\vec{x} \neq 0$ that $\vec{y}^* \vec{y} > 0$

6)

b)

So if **A is self-adjoint (symmetric) but not Positive Definite** then the algorithm will break because some square roots might be zero or undefined. Zero is also not allowed because the matrix R needs to have positive diagonal entires.

If **A is not self-adjoint but positve definite** the factorization will not work because it counts on A having mirrored entries.

For a simple 2×2 matrix

$$
\begin{pmatrix} 1 & 2 \\ 2 & -3 \end{pmatrix} = \begin{pmatrix} r_{11}^2 & r_{11} r_{12} \\ r_{11} r_{12} & r_{12}^2 + r_{22}^2 \end{pmatrix}
$$

It breaks down because you cant solve the

$$
r_{11} r_{12}
$$

line for two different solutions